Finite Size Corrections for the Pairing Hamiltonian

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Abstract

We study the effects of superconducting pairing in small metallic grains. We show that in the limit of large Thouless conductance one can explicitly determine the low energy spectrum of the problem as an expansion in the inverse number of electrons on the grain. The expansion is based on the formal exact solution of the Richardson model. We use this expansion to calculate finite size corrections to the ground state energy, Matveev-Larkin parameter, and excitation energies.

I. INTRODUCTION

Since mid 1990's, when Ralph, Black, and Tinkham succeeded in resolving the discrete excitation spectrum of nanoscale superconducting metallic grains[1], there has been considerable effort to describe theoretically superconducting correlations in such grains (see e.g. Ref. 2 for a review). A key question in any such description is how results of the BCS theory are modified in finite systems. In this paper we address this problem by developing a systematic expansion in the inverse number of electrons on the grain for the low energy spectrum of the problem.

In the absence of spin-orbit interaction and magnetic fields one can describe[3] superconducting correlations in weakly disordered grains by a simple pairing (BCS) Hamiltonian

$$H_{BCS} = \sum_{i,\sigma} \epsilon_i c_{i\sigma}^\dagger c_{i\sigma} - \lambda d \sum_{i,j=1}^{n} c_{i\downarrow}^\dagger c_{i\uparrow}^\dagger c_{j\uparrow} c_{j\downarrow} \qquad (1.1)$$

Here ϵ_i are orbital energy levels and d is the mean level spacing, $d = \langle \epsilon_{i+1} - \epsilon_i \rangle$. Operators $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) create (annihilate) an electron of spin projection σ in orbital state i, n is the total number of levels, and λ denotes a dimensionless coupling constant. The interaction part of Hamiltonian (1.1) allows only transitions of singlet electron pairs between the orbitals.

BCS Hamiltonian (1.1) is known to be integrable[4] and solvable by Bethe's *Ansatz*. The exact solution[5] yields a complicated set of coupled polynomial equations (see Eq. (1.2) bellow). As a consequence, very few explicit results have been derived and most studies resorted to numerics[2,6,7] based on the exact solution. The purpose of the present paper is to remedy this situation in the regime when the level spacing is the smallest energy scale in the problem.

BCS Hamiltonian (1.1) was studied extensively in 1960's in the context of pair correlations in nuclear matter[8]. A straightforward but important observation was that singly occupied orbitals do not participate in pair scattering[9]. Hence, the labels of these orbitals are good quantum numbers and their contribution to the total energy is only through the kinetic term in BCS Hamiltonian (1.1). Due to this "blocking effect" the problem of diagonalizing Hamiltonian (1.1) reduces to the subspace of orbitals that are either empty or doubly occupied – "unblocked" orbitals. The latter problem turns out to be solvable[5] by Bethe's *Ansatz*. The spectrum is obtained from the following set of algebraic equations for

unknown parameters E_i:

$$-\frac{1}{\lambda d} + \sum_{j=1}^{m}{}' \frac{1}{E_i - E_j} = \frac{1}{2}\sum_{k=1}^{n}\frac{1}{E_i - \epsilon_k} \quad i = 1,\ldots,m \tag{1.2}$$

where m is the total number of singlet pairs and n now is the number of unblocked orbitals ϵ_k. Bethe's *Ansatz* equations (1.2) for BCS Hamiltonian (1.1) are commonly referred to as Richardson's equations. Eigenvalues of BCS Hamiltonian (1.1) are related to Richardson parameters, E_i, via

$$E = 2\sum_{i=1}^{m}E_i + \sum_{B}\epsilon_B \tag{1.3}$$

where $\sum_B \epsilon_B$ is a sum over singly occupied – "blocked" orbitals.

In 1977, Richardson used exact solution (1.2) to outline[10] a method for expanding the low energy spectrum in powers of the inverse number of pairs, $1/m$. Richardson showed that BCS results[11] for the energy gap, condensation energy, excitation spectrum etc. are recovered from exact solution (1.2) in the thermodynamical limit. The proper limit is obtained by taking the number of levels, n, to infinity, so that $nd \to 2D = \text{const}, \; m = n/2$, where D is an ultraviolet cutoff usually identified with Debye energy. In particular, for equally spaced levels ϵ_i, the energy gap Δ and the ground state energy in the thermodynamical limit are

$$\Delta_0(\lambda) = \frac{D}{\sinh(1/\lambda)} \qquad E_{g.s.}^{BCS}(\lambda) = -Dm\coth 1/\lambda \tag{1.4}$$

In the present paper we show that the ground state and excitation energies of BCS Hamiltonian (1.1) can be evaluated explicitly to any order in $d/\Delta_0 \sim 1/m$ in terms of the BCS gap Δ_0, chemical potential μ, mean level spacing d, ultraviolet cutoff D, and the thermodynamic density of states $\nu(\epsilon)$. In the physical limit $\Delta_0/D \to 0$, the expansion is applicable for $\Delta_0 \geq d$. In fact, we believe that in this limit the expansion is in powers of d/Δ_0 with a convergence radius $d/\Delta_0 \sim 1$.

BCS Hamiltonian (1.1) supports two types of low energy excitations. Excitations of the first type preserve the number of pairs (pair-preserving excitations). The second type of low lying excitations (pair-breaking excitations) is obtained by breaking a single electron pair. In the thermodynamical limit both types of excitations are gapped with the same gap, $\Delta^p = \Delta^b = 2\Delta_0$, where Δ^p and Δ^b are the energy gaps for pair-preserving and pair-breaking excitations respectively. In Section V, we evaluate leading finite size corrections (of order $1/m$) to the gaps Δ^p and Δ^b. Interestingly, it turns out that these corrections coincide, even though the two gaps are not identical in higher orders in $1/m$. In the limit $\Delta_0/D \to 0$, our

result yields $\Delta^p = \Delta^b = 2\Delta_0 - d$. We also show that the energy levels of lowest excitations of two types cross at certain value of the coupling constant λ.

Another measure of the low energy properties of BCS model (1.1) is the parity parameter[12] introduced by Matveev and Larkin. This parameter is defined as

$$\Delta_{ML} = E_{g.s.}^{2m+1} - \frac{1}{2}\left(E_{g.s.}^{2m+2} + E_{g.s.}^{2m}\right) \tag{1.5}$$

where $E_{g.s.}^l$ is the ground state energy of BCS Hamiltonian (1.1) with l electrons. Matveev and Larkin evaluated Δ_{ML} in the physical limit $\Delta_0/D \to 0$ in two different regimes: $\Delta_0 \gg d$ and $\Delta_0 \ll d$. They found that in the first regime the leading finite size correction to the parity parameter (1.5) comes entirely from the stationary point (mean field) expression for the ground state energy of BCS Hamiltonian (1.1). Here we use our method to calculate Δ_{ML} in the regime $\Delta_0 > d$ for an arbitrary ratio Δ_0/D. We show that the contribution of quantum fluctuations to the leading finite size correction to Δ_{ML} behaves as $(\Delta_0/D)\ln(\Delta_0/D)$ for small Δ_0/D.

The ground state energy of pairing Hamiltonian (1.1) has been discussed recently in a number of papers. Numerical fits for finite size corrections to the ground state energy in the weak coupling regime, $\lambda \ll 1$, have been proposed[6,7]. Here we evaluate the leading finite size correction exactly and find a complete agreement with numerical results[6,7] in the weak coupling regime.

In Ref. 7, authors studied the condensation energy, defined as the difference between the ground state energy and the expectation value of BCS Hamiltonian (1.1) in the Fermi ground state. This difference was calculated in second order perturbation theory in λ and compared to BCS expression $E_{g.s.}^{BCS}(\lambda) - E_{g.s.}^{BCS}(0)$. The authors found that the two expressions become of the same order when $d \le \Delta_0 \le \sqrt{Dd}$ and interpreted this as a new, "intermediate", regime of pairing correlations in metallic grains. We argue bellow that, although the finite size correction to the condensation energy indeed becomes of the same order as the BCS result for $d \le \Delta_0 \le \sqrt{Dd}$, this fact does not indicate a new physical regime, but is rather an artifact of the model. Main contribution to the finite size correction to the condensation energy comes from energies close to the ultraviolet cutoff D and therefore is beyond limits of applicability of BCS Hamiltonian (1.1). Effects coming from this range of energies can be properly accounted for[13] within the Eliashberg theory[14].

The paper is organized as follows. Section II is devoted to the review of a general method[10]

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of $1/m$ expansion due to Richardson. In Section III, we show that Richardson's results can be used to evaluate ground state and excitation energies of BCS Hamiltonian (1.1) to any order in $1/m$ and explicitly calculate the leading correction to the ground state energy. In Section IV, we discuss various limits of our results and make a comparison with previous work. Results for the excitation spectrum and Matveev Larkin parameter are collected in Sections V and VI respectively, where we also determine the gaps for pair-breaking and pair-preserving excitations and discuss the range of applicability of the $1/m$ expansion.

II.   REVIEW OF RICHARDSON'S $1/m$ EXPANSION

Here we briefly review Richardson's $1/m$ expansion[10] for the ground state and excitation energies of pairing Hamiltonian (1.1). The details can be found in the original work[10]. In subsequent sections we will use Richardson's results to explicitly evaluate finite size corrections to the low energy spectrum of BCS Hamiltonian (1.1).

Richardson's $1/m$ expansion is based on an electrostatic analogy to equations (1.2). In this analogy, the roots E_i of equations (1.2) are interpreted as locations of m two-dimensional free charges of unit strength in the complex plane. The free charges are subject to a uniform external field $-1/(\lambda d)$ and the field of n fixed charges of strength $1/2$ located at the points ϵ_k on the real axis. The total electrostatic field at a point z associated with the charge distribution is given by

$$F(z) = \sum_{i=1}^{m} \frac{1}{z - E_i} - \frac{1}{2} \sum_{k=1}^{n} \frac{1}{z - \epsilon_k} - \frac{1}{\lambda d} \tag{2.1}$$

The field $F(z)$ contains complete information about the spectrum of BCS Hamiltonian (1.1). For example, the energy spectrum is related to the quadrupole momentum of $F(z)$. Indeed, defining multipole moments of $F(z)$ by

$$F(z) = \sum_{m=0}^{\infty} F^{(m)} z^{-m} \tag{2.2}$$

and expanding equation (2.1) in $1/z$, we obtain

$$E = 2 \sum_{i=1}^{m} E_i = 2F^{(2)} + \sum_{k=1}^{n} \epsilon_k \tag{2.3}$$

$$-\frac{1}{\lambda d} = F^{(0)} \tag{2.4}$$

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$$m - \frac{1}{2} = F^{(1)} \tag{2.5}$$

The $1/m$ expansion is facilitated by the following field equation that can be derived from equations (1.2) and (2.1):

$$\frac{dF}{dz} + F^2 = \frac{1}{2} \sum_k \frac{1}{(z - \epsilon_k)^2} + \frac{1}{4} \left(\sum_k \frac{1}{z - \epsilon_k} + \frac{2}{\lambda d} \right)^2 - \sum_k \frac{H_k}{z - \epsilon_k} \tag{2.6}$$

where H_k is the field at the location of the fixed charge ϵ_k due to the free charges

$$H_k = \sum_i \frac{2}{\epsilon_k - E_i} \tag{2.7}$$

Equation (2.6) can be solved by expanding the field $F(z)$ in powers of $1/m$

$$F(z) = \sum_{r=0}^{\infty} F_r(z) \tag{2.8}$$

where $F_r(z)$ is of order m^{1-r}. It turns out[10] that the lowest order in (2.8), $F_0(z)$, together with field equation (2.6) completely determine the field $F(z)$ to higher orders in $1/m$. Moreover, to obtain higher orders, $F_r(z)$ for $r \geq 1$, from $F_0(z)$ one needs to solve only algebraic equations.

Different states of the system are described by different $F_0(z)$. For example, one can show that the BCS ground state corresponds to

$$F_0(z) = -\sum_k \frac{\sqrt{(z - \mu)^2 + \Delta^2}}{2(z - \epsilon_k)\sqrt{(\epsilon_k - \mu)^2 + \Delta^2}} \tag{2.9}$$

The parameters Δ and μ correspond to the BCS gap and chemical potential respectively. Equations for Δ and μ can be derived by substituting $F_0(z)$ into equations (2.4) and (2.5)

$$\frac{2}{\lambda d} = \sum_k \frac{1}{\sqrt{(\epsilon_k - \mu)^2 + \Delta^2}} \tag{2.10}$$

$$n - 2m = \sum_k \frac{\epsilon_k - \mu}{\sqrt{(\epsilon_k - \mu)^2 + \Delta^2}} \tag{2.11}$$

There are no higher order corrections to equations (2.10) and (2.11), since by construction $F_0(z)$ yields exact monopole and dipole moments of $F(z)$, $F^{(0)}(z)$ and $F^{(1)}(z)$.

Note that, according to equations (2.1) and (2.9), $F_0(z)$ also describes the fixed charges exactly, since

$$\lim_{z \to \epsilon_k} (z - \epsilon_k) F_0(z) = -\frac{1}{2} \tag{2.12}$$

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Higher order corrections to the field $F(z)$ can be expressed only in terms of ϵ_k, Δ, μ and finite zeroes of $F_0(z)$

$$\sum_{k=1}^{n} \frac{1}{(x_l - \epsilon_k)\sqrt{(\epsilon_k - \mu)^2 + \Delta^2}} = 0 \tag{2.13}$$

For example,

$$F_1(z) = \frac{1}{2Z(z)} \left(\sum_k \frac{z + \epsilon_k - 2\mu}{Z(z) + Z(\epsilon_k)} - \sum_l \frac{z + x_l - 2\mu}{Z(z) + Z(x_l)} - \frac{z - \mu}{Z(z)} \right) \tag{2.14}$$

where

$$Z(z) = \sqrt{(z - \mu)^2 + \Delta^2}$$

One can show (by e.g. sketching the LHS of equation (2.13)) that there are $n - 1$ finite solutions to equation (2.13), each of them lying between two consecutive single electron levels ϵ_k.

The ground state energy to the first two orders in $1/m$, i.e. to the order m^0, can be obtained from $F_0(z)$ and $F_1(z)$ using equation (2.3).

$$E = E_0 + E_1$$

$$E_0 = \sum_k \epsilon_k - \mu(n - 2m) + \frac{\Delta^2}{\lambda d} - \sum_k \sqrt{(\epsilon_k - \mu)^2 + \Delta^2} \tag{2.15}$$

$$E_1 = -m\lambda d + \sum_{l=1}^{n-1} \left[\sqrt{(x_l - \mu)^2 + \Delta^2} - \frac{N_l}{P_l} \right] \tag{2.16}$$

where

$$N_l = \sum_k \frac{1}{(x_l - \epsilon_k)^2} \quad P_l = \sum_k \frac{1}{(x_l - \epsilon_k)^2 \sqrt{(\epsilon_k - \mu)^2 + \Delta^2}}$$

To calculate excitation energies one needs to appropriately modify $F_0(z)$, the lowest order in $1/m$ of the electrostatic field $F(z)$. Here we simply write down excitation energies to the first two nonzero orders in $1/m$ referring readers interested in the detailed derivation to the original work.[10]

$$e(l) = e_1(l) + e_2(l) \qquad l = 1, \ldots, n - 1$$

$$e_1(l) = 2\sqrt{(x_l - \mu)^2 + \Delta^2} \tag{2.17}$$

$$e_2(l) = 2 \sum_{m \neq l} \frac{1}{P_l} \left[(F_1')^2 - (F_1)^2 + \frac{d}{dz}(F_1' - F_1) + \frac{2F_1'}{x_m - x_l} \right]_{z = x_m} \tag{2.18}$$

where

$$F_1'(z) = F_1(z) + \frac{\sqrt{(x_l - \mu)^2 + \Delta^2}}{(z - x_l)\sqrt{(z - \mu)^2 + \Delta^2}} - \frac{1}{z - x_l} \tag{2.19}$$

and $e(l)$ is the excitation energy relative to the ground state.

Finally, we note that the lowest nonzero order of $1/m$ expansion, E_0 and $e_1(l)$ for the ground state and excitation energies, reproduces the mean field (BCS) results for pairing Hamiltonian (1.1). Therefore, the mean field for pairing Hamiltonian (1.1) is exact in the thermodynamical limit, while contributions E_1 and $e_2(l)$, equations (2.16) and (2.18), are leading finite size corrections to the thermodynamical limit.

III.   GROUND STATE ENERGY

Here we evaluate the leading finite size correction to the ground state energy of BCS Hamiltonian (1.1).

First, we note that, as shown in Appendix A, expression (2.16) for the finite size correction E_1 can be cast into a simpler form

$$E_1 = \lambda d \left(\frac{n}{2} - m \right) + \sum_{l=1}^{n-1} \sqrt{(x_l - \mu)^2 + \Delta^2} - \sum_{k=1}^{n} \sqrt{(\epsilon_k - \mu)^2 + \Delta^2} \qquad (3.1)$$

To facilitate comparison to the mean field BCS result (1.4), we assume bellow $n = 2m$ equally spaced single electron levels $\epsilon_k = (k - m - 1/2)d$ with energies ranging from $D = (m - 1/2)d$ to $-D$. It should be emphasized, however, that explicit results in terms of Δ, μ, and the density of states $\nu(\epsilon)$ can be equally well obtained for arbitrary continuous $\nu(\epsilon)$.

Since $n = 2m$ and ϵ_k are distributed symmetrically with respect to zero, equation (2.11) yields $\mu = 0$, while equations (2.10), (2.15), and (3.1) become

$$\frac{2}{\lambda d} = \sum_{k=1}^{2m} \frac{1}{\sqrt{\epsilon_k^2 + \Delta^2}} \qquad (3.2)$$

$$E_0 = \frac{\Delta^2}{\lambda d} - \sum_{k=1}^{2m} \sqrt{\epsilon_k^2 + \Delta^2} \qquad (3.3)$$

$$E_1 = \sum_{l=1}^{2m-1} \sqrt{x_l^2 + \Delta^2} - \sum_{k=1}^{2m} \sqrt{\epsilon_k^2 + \Delta^2} \qquad (3.4)$$

Equation (2.13) for x_l now reads

$$f(x_l) = \sum_{k=1}^{2m} \frac{1}{(x_l - \epsilon_k)\sqrt{\epsilon_k^2 + \Delta^2}} = 0 \qquad (3.5)$$

Since for each ϵ_k there is $\epsilon_{k'} = -\epsilon_k$, $f(z)$ is an odd function of z. Therefore, $x_l = 0$ is a solution of equation (3.5), while the remaining $n - 2 = 2m - 2$ nonzero solutions come

in pairs of x_l and $-x_l$. Let us label $m-1$ positive roots x_l with $l = 1, \ldots, m-1$ and relabel m positive single electron energies ϵ_k with $k = 0, 1 \ldots, m-1$. Then, we can rewrite equation (3.4) as

$$E_1 = \Delta - 2\sqrt{\frac{d^2}{4} + \Delta^2} + 2\sum_{l=1}^{m-1}\sqrt{x_l^2 + \Delta^2} - \sum_{k=1}^{m-1}\sqrt{\epsilon_k^2 + \Delta^2} \qquad (3.6)$$

where we have separated contributions to the summations of $x_l = 0$ and $\epsilon_k = \pm d/2$.

Because x_l is located between ϵ_l and $\epsilon_{l-1} = \epsilon_l - d$, we can write it as $x_l = \epsilon_l - \alpha_l d$, where $0 < \alpha_l < 1$. Expanding $\sqrt{x_l^2 + \Delta^2}$ in x_l in the vicinity of $x_l = \epsilon_l$ and bearing in mind that $d \approx D/m$ is of order $1/m$, we obtain

$$E_1 = -\Delta - 2\sum_{l=1}^{m-1}\frac{\alpha_l d}{\sqrt{\epsilon_l^2 + \Delta^2}} \qquad (3.7)$$

where we neglected terms of order $1/m$. With the same accuracy, we can replace the summation over k with an integration

$$E_1 = -\Delta - 2\int_0^D d\epsilon \frac{\epsilon\alpha(\epsilon)}{\sqrt{\epsilon^2 + \Delta^2}} \qquad (3.8)$$

Note that E_1 is indeed of order m^0 as it should be. The function $\alpha(\epsilon)$ is evaluated in Appendix B. The result, up to terms of order $1/m$, is

$$\alpha(\epsilon) = -\frac{1}{\pi}\text{arccot}\frac{1}{\pi}\ln\left[\frac{D\sqrt{\epsilon^2 + \Delta^2} - \epsilon\sqrt{D^2 + \Delta^2}}{D\sqrt{\epsilon^2 + \Delta^2} + \epsilon\sqrt{D^2 + \Delta^2}}\right] \qquad (3.9)$$

Introducing a new variable

$$x = \frac{1}{\pi}\ln\left[\frac{D\sqrt{\epsilon^2 + \Delta^2} - \epsilon\sqrt{D^2 + \Delta^2}}{D\sqrt{\epsilon^2 + \Delta^2} + \epsilon\sqrt{D^2 + \Delta^2}}\right] \qquad \epsilon = -\frac{D\Delta\sinh(\pi x/2)}{\sqrt{\Delta^2\cosh^2(\pi x/2) + D^2}}, \qquad (3.10)$$

we can cast expression (3.8) into a more convenient form

$$E_1 = -2\int_0^\infty \frac{dx}{\pi}\frac{\Delta\sqrt{\Delta^2 + D^2}}{(1 + x^2)\sqrt{\Delta^2 + D^2\left(\cosh(\pi x/2)\right)^{-2}}} \qquad (3.11)$$

To complete the evaluation of the ground state energy to order m^0, we also need to calculate the leading term, E_0 with the same accuracy. The first step is to replace summation in equations (2.10) and (3.3) with integrations according to the following formula:

$$d\sum_{j=n_1}^{n_2} f(jd) = \int_{n_1 d}^{n_2 d} dx f(x) + \frac{d}{2}\left[f(n_1 d) + f(n_2 d)\right] + o(1/m)$$

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Equations (2.10) and (3.3) now read

$$\frac{2}{\lambda} = \int_{-D}^{D} \frac{d\epsilon}{\sqrt{\epsilon^2 + \Delta^2}} + \frac{d}{\sqrt{\Delta^2 + D^2}} \tag{3.12}$$

$$E_0 = \frac{\Delta^2}{\lambda d} - \frac{1}{d} \int_{-D}^{D} d\epsilon \sqrt{\epsilon^2 + \Delta^2} - \sqrt{\Delta^2 + D^2} \tag{3.13}$$

The solution of equation (3.12) for Δ to order m^0 is obtained by dropping the second term on the RHS. Evaluating the integral, we obtain $\Delta_0 = D/[\sinh(1/\lambda)]$ in agreement with equation (1.4). To compute the correction of order $1/m$ to Δ, we substitute $\Delta = \Delta_0 + \delta\Delta$ into equation (3.12) and expand in $\delta\Delta$. Keeping only terms of order $1/m$, we find

$$\Delta = \Delta_0 + d\frac{\Delta_0}{2D} \tag{3.14}$$

Plugging Δ into equation (3.13) and using $\sqrt{\Delta_0^2 + D^2} = D\coth(1/\lambda)$, we obtain up to terms of order $1/m$

$$E_0 = -\left(m + \frac{1}{2}\right) D\coth(1/\lambda) \tag{3.15}$$

Note also that Δ in expression (3.11) for E_1 can be replaced by Δ_0 up to terms of order $1/m$. Thus, the ground state energy of BCS Hamiltonian (1.1) for m pairs and $n = 2m$ equally spaced levels is

$$E_{g.s.} = -D\coth(1/\lambda)\left[m + \frac{1}{2} + \phi(\lambda)\right] \tag{3.16}$$

where

$$\phi(\lambda) = 2\int_0^{\infty} \frac{dx}{\pi(1+x^2)} \frac{\cosh(\pi x/2)}{\sqrt{\cosh^2(\pi x/2) + \sinh^2(1/\lambda)}} \tag{3.17}$$

The plot of function $\phi(\lambda)$ is shown on Fig. 1.

The finite size correction to the mean field BCS result (1.4) is

$$E_{g.s.} = E_{g.s.}^{BCS} + E_{f.s.}, \qquad E_{f.s.} = -D\coth(1/\lambda)\left[\frac{1}{2} + \phi(\lambda)\right] \tag{3.18}$$

Note that $E_{f.s.}$ is different from E_1 given by equation (3.11) due to contribution of order m^0 from E_0.

Higher order corrections to the ground state energy can also be evaluated explicitly. The first step is to express them in terms of Δ and x_l following prescriptions of Ref. 10. Then, Δ and x_l have to be calculated to appropriate order in $1/m$ using methods of this section and Appendix B. Final results for higher order corrections will involve multiple integrations
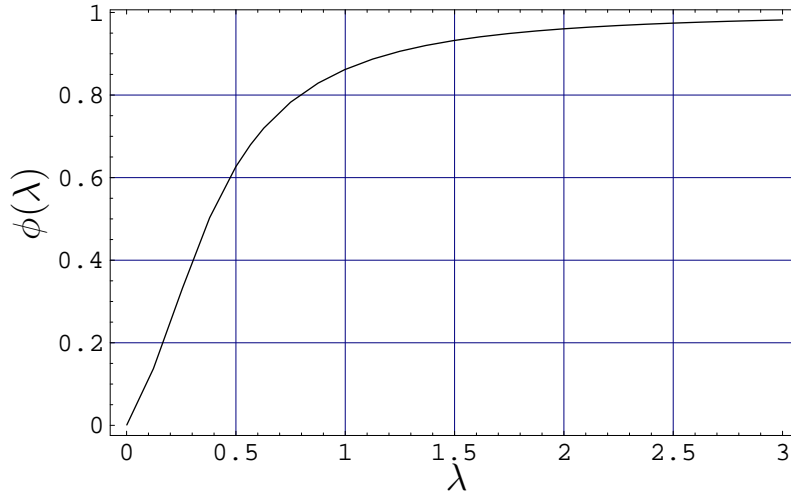
FIG. 1: The plot of function $\phi(\lambda)$ defined by equation (3.17). This function appears in leading finite size corrections to ground state (3.16) and excitation (5.10, 5.13) energies of BCS Hamiltonian (1.1) and to Matveev-Larkin parameter (6.2). Note the asymptotics $\phi(\lambda) \to 0$ and $\phi(\lambda) \to 1$ for $\lambda \to 0$ and $\lambda \to \infty$ respectively.

similar to the integration in equation (3.17). For example, the expression for the correction of order $1/m$ contains a triple integral.

The general case when the distribution of single electron levels in the limit $m, n \to \infty$, $m/n = $ fixed is described by a continuous density of states $\nu(\epsilon)$ can be treated similarly. Final expressions for corrections will now be in terms of Δ, μ, and $\nu(\epsilon)$. For example, the correction of order m^0 will be again given by the integral in equation (3.8) where the limits of integration should now be $-D$ and D, ϵ has to be replaced with $\epsilon - \mu$, and the integrand has to be multiplied by $\nu(\epsilon)$. The function $\alpha(\epsilon)$ will still be given by equation (B.2) where now $\nu(\epsilon)$ has to be included under the integral.

IV.   COMPARISON TO PREVIOUS STUDIES

Here we analyze our result and compare it to previous results. First, we check whether equation (3.18) reproduces the results of $1/\lambda$ expansion[15] around $\lambda = \infty$. Expanding the integrand in equation (3.17) in $1/\lambda$, evaluating the resulting integrals, and expanding

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$\coth(1/\lambda)$ in $1/\lambda$, we obtain

$$E_{f.s.} = -D\left[\frac{3}{2}\lambda + \frac{1}{3\lambda} - \frac{19}{360\lambda^2} + \frac{143}{15120\lambda^5} + O\left(\frac{1}{\lambda^7}\right)\right]$$

Comparing this expression with terms of order m^0 in $1/\lambda$ expansion[15] for the ground state energy (see equation (30) of Ref. 15), we find that the two results coincide.

Now let us consider the limit of small λ. The asymptotic behavior of $\phi(\lambda)$ for small λ is worked out in Appendix C. Here we write down the first two terms

$$\phi(\lambda) = \lambda + \ln 2 \cdot \lambda^2 + O(\lambda^3) \tag{4.1}$$

Expanding $\coth(1/\lambda) = \sqrt{1 + \Delta_0^2/D^2}$ in Δ_0/D and using $D = (m - 1/2)d$, we obtain from equation (3.16)

$$E_{g.s.} = -D\left(m + \frac{1}{2}\right) - \frac{\Delta_0^2}{2d} - D\lambda - \ln 2 \cdot D\lambda^2 + O(\lambda^3) \tag{4.2}$$

The first term in equation (4.2) is the energy of noninteracting Fermi ground state to order m^0. The second term is the nonperturbative mean field (BCS) contribution to the ground state energy. The first two terms are extensive and survive the thermodynamical limit. The last two terms give the correction to the ground state energy that one would obtain in the second order of ordinary perturbation theory in λ around noninteracting Fermi ground state.

We see that our result (3.18) yields the leading finite size correction to the thermodynamical limit for all values of λ. In particular, there is no breakdown in the regime of ultrasmall grains, i.e. for $d > \Delta_0$. As we will see in subsequent sections, this is not a generic feature of our approach, but is specific to the ground state energy and is probably related to the ultraviolet nature (see bellow) of the finite size correction calculated above.

A frequently discussed quantity[2,6,7] is the difference between the ground state energy and the expectation value of BCS Hamiltonian (1.1) in the unperturbed Fermi ground state, $|F.g.s.\rangle$, i.e. a state where single particle levels bellow the Fermi level, $\epsilon_k < 0$, are doubly occupied, while the remaining levels are empty. This difference is often called condensation energy, even though this name is misleading for the reasons detailed bellow. However, to facilitate a comparison with results of Ref. 6 and 7, we will use the same terminology in this section. We have

$$E_{cond.} = \langle F.g.s.|H_{BCS}|F.g.s.\rangle - E_{g.s.} = -D\left(m + \frac{1}{2}\right) - 2\lambda md - E_{g.s.}$$

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Using $D = (m - 1/2)d$ and equation (4.2), we obtain

$$E_{cond.} = \frac{\Delta_0^2}{2d} + \ln 2 \cdot D\lambda^2 + O(\lambda^3) \tag{4.3}$$

Comparison shows that the exact result (4.3) for $E_{cond.}$ to order m^0 is in complete agreement with fits to numerical data.[6,7]

Finally, note that the second term in expression (4.3) is ultraviolet divergent, since it depends explicitly on the ultraviolet cutoff D. For pairing by phonons the ultraviolet cutoff D can be identified with the Debye energy ω_D. To properly take into account any effect that comes from energies of the order of ω_D, one needs to go beyond the BCS theory which is appropriate only at energies much lower than ω_D. The contribution from these energies to finite size corrections can be adequately treated[13] within the Eliashberg theory[14]. In particular, the hard cutoff at $D = \omega_D$ has to be replaced by a soft effective cutoff due to the $1/\omega^2$ decay of the phonon propagator for frequencies $\omega \gg \omega_D$. Therefore, even though the contribution of the finite size correction in equation (4.3) becomes important for $\Delta_0 \leq \sqrt{Dd}$, the conclusion of Ref. 7 that this is an indication of any new physical regime is not justified.

V. EXCITATION ENERGIES

In this section we evaluate leading finite size corrections to lowest excitation energies. As we will see bellow, the results of this section are accurate only in the regime of relatively large grains, $\Delta_0 > d$, i.e. within terms of order $o(d/\Delta_0)$. These higher order corrections can also be straightforwardly calculated using methods of Sections III. However, we will only evaluate corrections of order d/Δ_0 here.

As in Section III, we will perform calculations for the case of $2m$ electrons and $n = 2m$ equally spaced levels $\epsilon_k = (k - m - 1/2)d$ with energies ranging from $D = (m - 1/2)d$ to $-D$. In this case, equation (2.11) implies $\mu = 0$. A more general case when the single electron levels are distributed with a smooth density of states can be treated similarly (see the discussion bellow equation (3.18)).

Note that Hamiltonian (1.1) conserves the number of paired electrons. Therefore, the excitations can be grouped into two types: those that preserve the number of pairs and those that break pairs. Energies of low lying pair-preserving excitations in the thermodynamical

limit are given by equation (2.17) with $\mu = 0$

$$e_1^p = 2\sqrt{x_l^2 + \Delta_0^2} \tag{5.1}$$

where x_l are the roots of equation (2.13). Low lying pair-breaking excitations are obtained by breaking a single pair and placing the two unpaired electrons on two single electron levels ϵ_a and ϵ_b. The energy of this excitation according to equation (1.3) is

$$e^b = \epsilon_a + \epsilon_b + E_{g.s.}(\epsilon_a, \epsilon_b) - E_{g.s.} \tag{5.2}$$

where $E_{g.s.}(\epsilon_a, \epsilon_b)$ is the ground state energy of BCS Hamiltonian (1.1) with levels ϵ_a and ϵ_b blocked. In the thermodynamical limit, using equation (2.15), we obtain

$$e_1^b = \sqrt{\epsilon_a^2 + \Delta_0^2} + \sqrt{\epsilon_b^2 + \Delta_0^2} \tag{5.3}$$

Therefore, in the thermodynamical limit both types of excitations are gapped with the same gap $2\Delta_0$, i.e.

$$\Delta_1^p = \Delta_1^b = 2\Delta_0 \tag{5.4}$$

Since pair-breaking excitations are capable of carrying spin-1, Δ^b can also be called the spin gap. To calculate corrections to Δ_1^p and Δ_1^b, one needs to go beyond mean field approximation.

First, let us determine the energy of lowest lying pair-breaking excitations to order $1/m$. Breaking a pair changes both the number of pairs to $m' = m - 1$ and also the number of unblocked levels to $n' = 2m - 2 = 2m'$. The lowest energy is archived by blocking levels $\epsilon_a = d/2$ and $\epsilon_b = -d/2$. Since this leaves the distribution of single particle levels symmetric with respect to zero, the chemical potential μ in equation (2.11) remains equal to zero, $\mu' = \mu = 0$. However, the blocking affects the gap Δ', since now terms corresponding to $\epsilon_k = \pm d/2$ have to be excluded from gap equation (2.10). Using equation (2.10), we obtain

$$\sum_k \frac{1}{\sqrt{\epsilon_k^2 + \Delta'^2}} = \frac{2}{\sqrt{d^2/4 + \Delta^2}} + \sum_k \frac{1}{\sqrt{\epsilon_k^2 + \Delta^2}} \tag{5.5}$$

where Δ' is the value of the gap with levels $\pm d/2$ blocked. Expanding the LHS of equation (5.5) in $\delta\Delta = \Delta' - \Delta$ and using gap equation (2.10), we obtain

$$\delta\Delta = -d\sqrt{1 + \frac{\Delta^2}{D^2}} \tag{5.6}$$

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According to equation (5.2), to order $1/m$ the lowest lying pair-breaking excitations have the following energy:

$$\Delta^b = E_0'(\Delta') - E_0(\Delta) + E_1'(\Delta', x_l') - E_1(\Delta, x_l) \tag{5.7}$$

where $E_0(\Delta)$ and $E_1(\Delta, x_l)$ are given by equations (3.3) and (3.4) respectively and primes denote quantities for the ground state with levels $\pm d/2$ blocked. Equations (3.3), (3.4), (5.6), and (3.14) imply

$$E_0'(\Delta') - E_0(\Delta) = 2\Delta' + \sum_k \frac{\delta\Delta\Delta}{4(\epsilon_k^2 + \Delta^2)^{3/2}} = 2\Delta_0 + \frac{d\Delta_0}{D} - d\sqrt{1 + \frac{\Delta_0^2}{D^2}} \tag{5.8}$$

$$E_1'(\Delta', x_l') - E_1(\Delta, x_l) = \frac{\partial E_1(\Delta)}{\partial \Delta}\delta\Delta + \sum_l \frac{x_l \delta x_l}{\sqrt{x_l^2 + \Delta^2}} \tag{5.9}$$

where $E_1(\Delta)$ is given by equation (3.11) and δx_l is the change in x_l due to blocking levels $\pm d/2$.

We see from equation (3.5) that the effect of removing levels $\epsilon_k = \pm d/2$ from the summation in equation (2.13) is strongest for the roots closest to the blocked levels $\pm d/2$. For these roots $\delta x_l \sim d$. On the other hand, due to an additional factor of x_l in front of δx_l in equation (5.9), the contribution of each of these x_l to the RHS of equation (5.9) is of order d^2/Δ. By splitting the sum in equation (3.5) into two sums as in Appendix B, one can show that the contribution of all these roots to the sum in equation (5.9) is of order $o(1/m)$. For the remaining roots, $\delta x_l/x_l$ is of order $1/m$ and each term in equation (3.5) can be expanded into $\delta x_l/(x_l - \epsilon_k)$. We have

$$\sum_{\epsilon_k \neq \pm d/2} \frac{1}{\sqrt{\epsilon_k^2 + \Delta^2}(x_l' - \epsilon_k)} = \sum_{k=1}^{2m} \frac{1}{\sqrt{\epsilon_k^2 + \Delta^2}(x_l + \delta x_l - \epsilon_k)} - \frac{2}{x_l \Delta} = \sum_{k=1}^{2m} \frac{1}{\sqrt{\epsilon_k^2 + \Delta^2}(x_l - \epsilon_k)}$$

Expanding into δx_l, we obtain

$$\delta x_l \sum_k \frac{1}{\sqrt{\epsilon_k^2 + \Delta^2}(x_l - \epsilon_k)^2} = -\frac{2}{x_l \Delta}$$

The summation here can be evaluated in the same way as the first sum in equation (B.1) of Appendix B is evaluated. Recall that roots of equation (3.5) x_l and therefore δx_l are distributed symmetrically with respect to zero. Using the notation introduced in the text following equations (3.5) and (3.6), we have for $x_l > 0$

$$\delta x_l x_l = -\frac{2d^2\sqrt{\epsilon_l^2 + \Delta^2}}{\Delta}\frac{\sin^2 \pi\alpha(\epsilon_l)}{\pi^2}$$

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where $\alpha(\epsilon_l)$ is given by equation (3.9). Substituting $\delta x_l x_l$ into equation (5.9) and using equations (5.8), (5.7), (3.9), and (3.11), we obtain

$$\Delta^b = 2\Delta_0 - d\sqrt{1 + \frac{\Delta_0^2}{D^2}} + \frac{d\Delta_0}{D}\left[1 + \phi(\lambda)\right] \tag{5.10}$$

where we used the change of variables (3.10) and $\phi(\lambda)$ is defined by equation (3.17). Expression (5.10) yields the energy of lowest lying pair-breaking excitations up to terms of order $o(d/(\min[D, \Delta_0]))$.

In the physical limit of weak coupling, $\Delta_0/D \to 0$, according to equation (4.1), expression (5.10) becomes

$$\Delta^b = 2\Delta_0 - d + o(d/\Delta_0) \tag{5.11}$$

Next, we turn to excitations that preserve the number of pairs. Energies of these excitations to order $1/m$ are given by equations (2.17) and (2.18). Equation (5.1) shows that the lowest lying excitation corresponds to $x_l = 0$. We have, up to terms of order $o(d/(\min[D, \Delta_0]))$

$$\Delta^p = 2\Delta + 2 \sum_{x_m \neq 0} \frac{1}{P_l}\left[(F_1')^2 - (F_1)^2 + \frac{d}{dz}(F_1' - F_1) + \frac{2F_1'}{x_m}\right]_{z=x_m} \tag{5.12}$$

where $F_1(z)$ and $F_1'(z)$ are defined by equations (2.14) and (2.19). Taking into account that both ϵ_k and x_l are distributed symmetrically with respect to zero and $\mu = 0$, we can rewrite these equations as

$$F_1(z) = \frac{z}{2\sqrt{z^2 + \Delta^2}}\left(\sum_k \frac{1}{\sqrt{z^2 + \Delta^2} + \sqrt{\epsilon_k^2 + \Delta^2}} - \sum_l \frac{1}{\sqrt{z^2 + \Delta^2} + \sqrt{x_l^2 + \Delta^2}} - \frac{1}{\sqrt{z^2 + \Delta^2}}\right)$$

$$F_1'(z) = F_1(z) + \frac{\sqrt{x_l^2 + \Delta^2}}{(z - x_l)\sqrt{z^2 + \Delta^2}} - \frac{1}{z - x_l}$$

Summations in $F_1(z)$ and in equation (5.12) can be evaluated in the same way as sums in equations (5.9) and (3.6) have been evaluated. Even though this calculation looks rather different from the one that lead to equation (5.10), it yields an identical result, i.e.

$$\Delta^p = \Delta^b + o(d/(\min[D, \Delta_0])) \tag{5.13}$$

Thus, both gaps coincide up to terms of order $o(1/m)$. However, this coincidence is not preserved in higher orders. Indeed, it was shown in Ref. 15 that in the strong coupling limit, $\lambda \gg 1$, the gap for pair-breaking excitations is larger $\Delta^b - \Delta^p \simeq d^2/\Delta_0 > 0$. On

the other hand, at $\lambda = 0$ the gap for pair-preserving excitations is larger, $\Delta^b - \Delta^p = -d$. Therefore, the lowest energy levels of the two types of excitations cross at certain value of Δ_0. Equation (5.13) shows that the distance between the two levels is reduced from d at Δ_0 to $o(d/\Delta_0) d$ even when $d \ll \Delta_0 \ll D$. However, the knowledge of higher order corrections to the gaps Δ^b and Δ^p is needed to determine whether the crossing occurs in the physical regime $\Delta_0/D \to 0$, i.e. at $\Delta_0 \simeq d$.

VI. MATVEEV-LARKIN PARAMETER

Finally, let us evaluate the Matveev-Larkin parameter[12]. This parameter is a measure of a parity effect in the grain and is defined as follows:

$$\Delta_{ML} = E_{g.s.}^{2m+1} - \frac{1}{2}\left(E_{g.s.}^{2m+2} + E_{g.s.}^{2m}\right) \tag{6.1}$$

where $E_{g.s.}^l$ is the ground state energy of BCS Hamiltonian (1.1) with l electrons.

The calculation of Δ_{ML} is similar to the one that lead to equation (5.10), only now we also have to take into account the change in the chemical potential

$$\mu_{2m+2} - \mu_{2m} = 2(\mu_{2m+1} - \mu_{2m}) = -2(\Delta_{2m+2} - \Delta_{2m}) = d\sqrt{1 + \frac{\Delta_0^2}{D^2}}$$

$$\Delta_{2m+2} - \Delta_{2m} = O(d^2/\Delta_0)$$

The calculation results in

$$\Delta_{ML} = \frac{\Delta^b}{2} = \Delta_0 - \frac{d}{2}\sqrt{1 + \frac{\Delta_0^2}{D^2}} + \frac{d\Delta_0}{2D}\left[1 + \phi(\lambda)\right] \tag{6.2}$$

where $\phi(\lambda)$ is defined by equation (3.17). As before, this expression is accurate up to terms of order $o(d/(\min[\Delta_0, D]))$. In the physical limit $\Delta_0/D \to 0$, expression (6.2), according to equation (4.1), reduces to the one obtained in Ref. 12

$$\Delta_{ML} = \Delta_0 - \frac{d}{2} + o(d/\Delta_0) \tag{6.3}$$

The first three terms on the RHS of equation (6.2) come from the mean field (stationary point) approximation (2.15) for the ground state energy. The last term in equation (6.2) represents the contribution of order $1/m$ of quantum fluctuations around the stationary point. The asymptotic behavior of this term in the physical limit $\Delta_0/D \to 0$ is given by

equation (4.1). In terms of d, Δ_0, and D it reads $d\ln(\Delta_0/D)\Delta_0/D$. In this limit quantum fluctuations will contribute to higher orders in d/Δ_0 as evidenced by the result[12] for Δ_{ML} in the regime $d \ll \Delta_0$. Therefore, it is of certain interest to use methods of Section III to evaluate further corrections to Δ_{ML}.

We conclude this section with a comment on the range of applicability of $1/m$ expansion detailed in this paper. It is clear from equations (5.11) and (6.3) that the expansion is applicable in the regime $\Delta_0 \geq d$. In fact, results of Ref. 15 and 10 (see also Section II) suggest that the expansion is in powers of d/Δ_0 with a convergence radius $d/\Delta_0 \simeq 1$.

VII.   CONCLUSION

In this paper we have shown that finite size corrections to the thermodynamical limit for pairing Hamiltonian (1.1) can be evaluated explicitly in terms of the BCS gap Δ_0, chemical potential μ, mean level spacing d, ultraviolet cutoff D, and the thermodynamic density of states $\nu(\epsilon)$ to any order in $d/\Delta_0 \sim 1/m$.

We evaluated leading corrections to the ground state and lowest excitation energies, and to Matveev-Larkin parameter (equations (3.18, 5.10, 5.11, 5.13, 6.2, 6.3)). Our results for the ground state energy are in agreement with previous numerical studies. We showed that the finite size correction to the condensation energy is ultraviolet divergent and therefore comparing it to the BCS result is not justified.

We found that the gaps for pair-breaking and pair-conserving excitations of pairing Hamiltonian (1.1) coincide up to terms of order $o(1/m)$, where m is the number of electron pairs on the grain. In higher orders in $1/m$ the two gaps are different, the difference being of order d^2/Δ_0, where d is the mean level spacing and Δ_0 is the BCS gap (1.4). We showed that the energy levels of the lowest excitations of two types cross at a certain value of the coupling constant λ.

The range of applicability of $1/m$ expansion detailed in the present paper is $\Delta_0 \geq d$. In fact, we believe that in the physical limit $\Delta_0/D \to 0$ the expansion is a power series in d/Δ_0 with a convergence radius of order one.

Note that our results significantly simplify in the physical limit $\Delta_0/D \to 0$ (e.g. compare equations (5.10) and (5.11)). An interesting open problem is to take this limit directly in Richardson's equations (1.2) and to develop a simplified version of the $1/m$ expansion for

this case. In particular, this might help to address the problem of the crossover between the fluctuation dominated ($d \gg \Delta_0$) and the bulk ($d \ll \Delta_0$) regimes.

VIII.   ACKNOWLEDGEMENTS

IX.   APPENDIX A

Here we show that expression (2.16) for the correction to the ground state energy can be simplified to equation (3.1). Indeed, define

$$f(z) = \sum_{k=1}^{n} \frac{d_k}{z - \epsilon_k} \qquad \text{where } d_k = \frac{1}{\sqrt{(\epsilon_k - \mu)^2 + \Delta^2}}$$

Equation (2.13) now reads $f(x_l) = 0$. The function $f(z)$ has $n - 1$ finite zeroes at $z = x_l$ and also a zero at $z = \infty$. Its dual function, $g(z) = 1/f(z)$, has $n - 1$ poles at $z = x_l$ and also a pole at $z = \infty$ with a residue $(\sum_{k=1}^{n} d_k)^{-1}$. Therefore, it can be represented as

$$g(z) = \sum_{l=1}^{n-1} \frac{m_l}{z - x_l} + \frac{z}{\sum_k d_k} = \sum_{l=1}^{n-1} \frac{m_l}{z - x_l} + \frac{\lambda d z}{2}$$

where we have used $\sum_k d_k = 2/(\lambda d)$ in accordance with gap equation (2.10). The following equations for the residues of $g(z)$ and $f(z)$ are helpful:

$$m_l = \lim_{z \to x_l} [(z - x_l)g(z)] = \lim_{z \to x_l} \frac{z - x_l}{f(z)} = \frac{1}{f'(x_l)} = -\left[\sum_k \frac{d_k}{(x_l - \epsilon_k)^2} \right]^{-1} = -\frac{1}{P_l}$$

$$\frac{1}{d_k} = \frac{1}{\lim_{z \to \epsilon_k} [(z - \epsilon_k)f(z)]} = g'(\epsilon_k) = -\sum_l \frac{m_l}{(x_l - \epsilon_k)^2} + \frac{\lambda d}{2}$$

where the prime denotes the derivative with respect to z. Using these equations, we obtain

$$\sum_{l=1}^{n-1} \frac{N_l}{P_l} = -\sum_{l=1}^{n-1} \sum_{k=1}^{n} \frac{m_l}{(x_l - \epsilon_k)^2} = \sum_{k=1}^{n} \left(\frac{1}{d_k} - \frac{\lambda d}{2} \right) = -\frac{\lambda d n}{2} + \sum_{k=1}^{n} \sqrt{(\epsilon_k - \mu)^2 + \Delta^2} \qquad \text{(A.1)}$$

Finally, substituting equation (A.1) into expression (2.16), we obtain equation (3.1).

X.   APPENDIX B

In this Appendix we solve equation (3.5) for x_l. As was discussed bellow equation (2.14), each solution x_l lies between two consecutive single electron levels ϵ_k. Consider the solution $x(\epsilon)$ that lies between $\epsilon - d$ and ϵ, where we dropped subscripts for simplicity.

Now let us multiply equation (3.5) by d and rewrite it as

$$\sum_{|\epsilon_k - \epsilon| \leq Jd} \frac{d}{(x(\epsilon) - \epsilon_k)\sqrt{\epsilon_k^2 + \Delta^2}} + \sum_{|\epsilon_k - \epsilon| > Jd} \frac{d}{(x(\epsilon) - \epsilon_k)\sqrt{\epsilon_k^2 + \Delta^2}} = 0 \qquad (B.1)$$

where $1 \ll J \ll \Lambda = \min[\Delta, D]/d$. For example, one can choose $J = \sqrt{\Lambda}$. In the first summation in equation (B.1), $\sqrt{\epsilon_k^2 + \Delta^2}$ can be replaced by $\sqrt{\epsilon^2 + \Delta^2}$ with a relative error of order Jd/Δ. We obtain

$$\sum_{|\epsilon_k - \epsilon| \leq Jd} \frac{d}{(x(\epsilon) - \epsilon_k)\sqrt{\epsilon_k^2 + \Delta^2}} = \left[1 + O\left(\frac{Jd}{\Delta}\right)\right] \frac{1}{\sqrt{\epsilon^2 + \Delta^2}} \sum_{p=0}^{J} \left[\frac{1}{p + 1 - \alpha(\epsilon)} - \frac{1}{p + \alpha(\epsilon)}\right]$$

where $\alpha(\epsilon)$ is defined by $x(\epsilon) = \epsilon - \alpha(\epsilon)d$. To determine $\alpha(\epsilon)$ to the leading (m^0) order in $1/m$, we can now take the limit $m \to \infty$. With a suitable choice of J (e.g. $J = \sqrt{\Lambda}$), $J \to \infty$ and $(Jd)/D \to 0$ in this limit, while the second sum in equation (B.1) becomes a principal value integral. Using,

$$\sum_{p=0}^{\infty} \left[\frac{1}{p + 1 - \alpha(\epsilon)} - \frac{1}{p + \alpha(\epsilon)}\right] = -\pi \cot(\pi \alpha(\epsilon))$$

we obtain

$$\pi \cot(\pi \alpha(\epsilon)) = \int_{-D}^{D} \frac{d\epsilon'}{(\epsilon - \epsilon')\sqrt{\epsilon'^2 + \Delta^2}} \qquad (B.2)$$

Finally, evaluating the integral, we arrive at equation (3.9).

Corrections $\delta\alpha(\epsilon)$ to $\alpha(\epsilon)$ of order $1/m$ and higher can also be evaluated explicitly by expanding equation (3.5) in $\delta\alpha(\epsilon)$. These corrections contribute to terms of order $1/m$ and higher in the ground state energy.

XI.   APPENDIX C

Here we determine the asymptotic behavior for small λ of the integral

$$\phi(\lambda) = 2 \int_0^{\infty} \frac{dx}{\pi(1 + x^2)} \frac{\cosh(\pi x/2)}{\sqrt{\cosh^2(\pi x/2) + \sinh^2(1/\lambda)}}$$

First, we note that up to terms of order $e^{-1/\lambda}$, one can rewrite this integral as

$$\phi(\lambda) = 2 \int_{-\infty}^{\infty} \frac{dx}{\pi[1 + (x + x_0)^2]\sqrt{1 + e^{-\pi x}}} \qquad \text{where } x_0 = \frac{2}{\pi\lambda}$$

Let us divide the domain of integration into three intervals: $(-\infty, -a)$, $(-a, a)$, and (a, ∞), where $1 \ll a \ll x_0$, and denote the corresponding integrals by I_3, I_2, and I_1 respectively. Each of the integrals I_k can be expanded into its own small parameter that depends on a. The dependence on a will cancel out when the results are added together. We have

$$I_3 = 2 \int_a^{\infty} \frac{dx}{\pi[1 + (x - x_0)^2]\sqrt{1 + e^{\pi x}}} = 2 \int_a^{\infty} \frac{dx}{\pi} \frac{e^{-\pi x/2} - e^{-3\pi x/2} + \cdots}{1 + (x - x_0)^2} = O(e^{-\pi a/2})$$

$$I_2 = 2 \int_{-a}^{a} \frac{dx}{\pi[1 + (x_0 + x)^2]\sqrt{1 + e^{-\pi x}}} = \frac{2}{x_0^2} \int_{-a}^{a} \frac{dx}{\pi\sqrt{1 + e^{-\pi x}}} -$$

$$\frac{2}{x_0^3} \int_{-a}^{a} \frac{x\,dx}{\pi\sqrt{1 + e^{-\pi x}}} + \ldots = \frac{2\pi a + 4\ln 2}{\pi^2 x_0^2} + O\left(\frac{a^2}{x_0^3}\right)$$

$$I_1 = 2 \int_a^{\infty} \frac{dx}{\pi[1 + (x + x_0)^2]\sqrt{1 + e^{\pi x}}} = 2 \int_a^{\infty} \frac{dx}{\pi} \frac{1 - e^{-\pi x}/2 + \cdots}{1 + (x + x_0)^2} = \frac{2}{\pi x_0} - \frac{2a}{\pi x_0^2} + O\left(\frac{a^2}{x_0^3}\right)$$

Adding I_1, I_2, and I_3, we obtain equation (4.2). Higher order terms can also be calculated by the same method.

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